The Ihara Zeta function and Quantum Walk (Profinite monodromy, Galois representations, and Complex functions)

Sato, Iwao

数理解析研究所講究録 第2120巻 2019年 199-219

The Ihara Zeta function and Quantum Walk

Iwao Sato
National Institute of Technology, Oyama College

Dedicated to Professor Yasutaka Ihara for the 80 birthday

Abstract

After Professor Ihara defined the Ihara zeta function in 1966, the Ihara zeta function was studied in various fields: number theory, algebra, random walk, combinatorics, graph theory, quantum graph, quantum walk, Ising model etc. The Ihara zeta function has four expressions: the Euler product, the exponential generating function, the determinant expression of Hashimoto type, the determinant expression of Ihara type. The determinant expression of Ihara type for the Ihara zeta function discovered by Professor Ihara is a marked one of it, and involves extremely many informations.

In this talk, we state determinant expressions of Ihara type for the Ihara zeta function of a graph and its variations, and then consider the relation between the Ihara zeta function and quantum walk from viewpoint of their determinant expressions of Ihara type. Recently, it turned out that discrete-time quantum walks on graphs are efficient for the graph isomorphism problem, and various approach are done in the graph isomorphism problem. Emms et al decided spectra for the Grover transition matrix of the Grover walk on a graph, its positive support and the positive support of its square, and so showed that the positive support of the third power of the Grover transition matrix outperforms the graph spectra methods in distinguishing strongly regular graphs. Furthermore, it is found out that the Grover transition matrix is closely related to the edge matrix appeared in the determinant expression of Hashimoto type for the Ihara zeta function of a graph. We determine the characteristic polynomials of them by using the determinant expressions of Ihara type for the Ihara zeta function and the second weighted zeta function of a graph, and directly present spectra for them. Furthermore, we state the structure of the positive support of the n th power of the Grover transition matrix.

1 Definition of Ihara zeta function

1.1 History

1. *1966, Ihara [22]: On discrete subgroups of the two by two projective linear group over p-adic fields, J. Math. Soc. Japan 18 (1966), 219-235.*

   Professor Ihara defined a p-adic Selberg zeta function (the *Ihara-Selberg zeta function* or the *Ihara zeta function*) to count the conjugacy classes of some discrete subgroup of $PGL(2, F)$ over a p-adic field F, and gave its *determinant expression of Ihara type* (*Ihara Theorem*).

2. *1980, Serre* [35]: Serre pointed out that the Ihara zeta function is a zeta function of some regular graph.

3. *1986, Sunada* [38]: Sunada gave the *definition* of the Ihara zeta function *by using terminologies of graph theory* and the *graph theoretic proof* of Ihara Theorem.

4. *1990, Hashimoto* [18]: Hashimoto gave the *determinant expression of Hashomoto type* for the Ihara zeta function of a general graph by using the *edge matrix*.

5. *1992, Bass* [4]: Bass gave the determinant expression of Ihara type for the Ihara zeta function of a general graph by using the *adjacency matrix*.

1.2 The original definition of the Ihara zeta function

Professor Ihara defined the Ihara zeta function in general situation([22]). Also, Professor Ihara studied Ihara zeta function in papers [20,21].

Let G be an abstract group. Then, for $x \in G$, the *length* $\ell(x) \in \mathbb{N}$ of x is defined as follows:

- (G, ℓ, I): for $\ell = 0, 1, 2, \ldots$,

$$G_\ell \neq \phi, U = G_0 < G(subgroup)$$

  and

$$G_\ell^{-1} = G_\ell, UG_\ell U = G_\ell, |U \setminus G_\ell| < \infty (\ell = 0, 1, 2, \ldots),$$

- (G, ℓ, II):

$$|U \setminus G_1| = q + 1$$

and

1. $G_1^2 = G_2 + (q+1)U$,
2. $G_1 G_\ell = G_{\ell+2} + qG_{\ell-1} (\ell \geq 2)$.

Next, let Γ be a subgroup of G such that

1. (Γ I) Γ is torsion-free and $\Gamma \cap x^{-1}Ux = \{1\}, \forall x \in G$,
2. (Γ II) $|U \setminus G/\Gamma| < \infty$.

Then note that Γ *is isomorphic to a free group with finite number of generators.*

Example

Let $G = PGL(2, k) = GL(2, k)/k^*$, where k is a locally compact field under a discrete valuation. Furthermore, let $\mathcal{O}(\mathcal{P})$ be a ring of integers (prime ideal) of k. For $x \in G$, we can choose a *matrix* $(a_{ij})_{1 \leq i,j \leq 2}$ such that

$$a_{ij} \in \mathcal{O} \ and \ \sum_{i,j=1}^{2} a_{ij}\mathcal{O} = \mathcal{O}.$$

Set

$$\det(a_{ij})\mathcal{O} = \mathcal{P}^{\ell(x)}.$$

Then G and ℓ satisfy (G, ℓ, I,II) by $q = N\mathcal{P}$ and $U = PGL(2, \mathcal{O}) = GL(2, \mathcal{O})/\mathcal{O}^*$

For any conjugacy class $\{\gamma\} \neq \{1\}$ of Γ, let

$$\deg\{\gamma\} = \min_{x \in G} \ell(x^{-1}\gamma x) > 0.$$

An element $\gamma \neq 1 \in \Gamma$ or a conjugacy class $\{\gamma\} \neq \{1\}$ is *primitive* if

$$C_\Gamma(\gamma) = \langle\gamma\rangle = \{x \in G \mid x^{-1}\gamma x = \gamma\},$$

where $C_\Gamma(\gamma)$ is the centralizer of γ in Γ.

Professor Ihara counted the number of primitive conjugacy classes of Γ.

Definition 1 (Ihara, 1966) *The* Ihara zeta function *is defined as follows:*

$$Z_\Gamma(u) = \prod_P (1 - u^{\deg P})^{-1},$$

where P runs over all primitive conjugacy classes of Γ.

Ihara presented the following result:

$$\log Z_\Gamma(u) = \sum_{P, m \geq 1} \frac{u^{m \deg P}}{m} = \sum_{m=1}^{\infty} \frac{N_m}{m} u^m, N_m = \sum_{\deg P | m} \deg P.$$

Professor Ihara considered more general situation([22]).

Let ρ be a finite dimensional representation of Γ over a field of characteristic 0. Furthermore, let

$$\chi(\gamma) = \mathrm{Tr}\rho(\gamma), \gamma \in \Gamma.$$

Definition 2 (Ihara, 1966) *The* Ihara L-function *is defined as follows:*

$$\begin{cases} \log Z_\Gamma(u, \chi) = \sum_{P, m \geq 1} \frac{\chi(P^m) u^{m \deg P}}{m} = \sum_{m=1}^{\infty} \frac{N_{m,\chi}}{m} u^m \\ \log Z_\Gamma(0, \chi) = 1. \end{cases}$$

Then note that

$$Z_\Gamma(u, \chi) = \prod_P \det(I_d - \rho(P) u^{\deg P})^{-1}, d = \deg \rho.$$

Now, we state the determinant expression for the Ihara L-function. Let

$$G = \sum_{i=1}^{h} U x_i \Gamma \ (h = |U \setminus G/\Gamma), S_{ij}^{(\ell)} = x_i^{-1} G_\ell x_j \cap \Gamma, \ S_{ij} = S_{ij}^{(1)} (\ell \geq 0; 1 \leq i, j \leq h).$$

Then it is known that ρ is extened to a representation of $\mathbb{Z}(\Gamma)$:

$$\rho(G_\ell) = A_\ell^\chi = (\sum_{\gamma \in S_{ij}^{(\ell)}} \rho(\gamma))(\ell \geq 0).$$

Here, note that

$$\deg \rho = \chi(1) h.$$

The determinant expression for the Ihara L-function is given as follows.

Theorem 1 (Ihara, 1966)

$$Z_\Gamma(u, \chi) = (1 - u^2)^{-g_\chi} \det(I_d - A_1^\chi u + q u^2)^{-1}, \tag{1}$$

where $g_\chi = (q-1) h \chi(1)/2$ and $d = \chi(1) h$.

In the case of $\rho = 1$,

$$Z_\Gamma(u) = (1 - u^2)^{-(q-1)h/2} \det(I_h - A_1 u + q u^2)^{-1}, \tag{2}$$

where

$$A_1 = (a_{ij}) : a_{ij} = |x_i^{-1} G_1 x_j \cap \Gamma| (1 \leq i, j \leq h).$$

The right sides are called the *determinant expressions of Ihara type.*

In the case that $G = PGL(2, k)$, $U = PGL(2, \mathcal{O})$ and Γ is a torsion-free discrete subgroup of G, $T = G/U$ is the $(q+1)$-*regular tree* and $K = \Gamma \setminus T = \Gamma \setminus G/U$ is a finite $(q+1)$-regular graph. Furthermore, T is the *universal covering* of K and $\Gamma = \pi_1(K)$. Serre pointed out that the Ihara zeta function $Z_\Gamma(u)$ is a zeta function of a $(q+1)$-regular graph K. From this consideration, Sunada defined the Ihara zeta function for $PGL(2, k)$ by using the terminologies of graph theory. In the next section, we state this definition.

1.3 The definition of the Ihara zeta function by the terminologies of graph theory

Let $G = (V(G), E(G))$ be a finite (simple) connected graph and D_G the symmetric digraph corresponding to G. Then D_G is the digraph obtained from G by replacing each edge $uv \in E(G)$ two directed edges (*arcs*) $(u, v), (v, u)$. Set $D(G) = \{(u, v), (v, u) \mid uv \in E(G)\}$. For $e = (u, v) \in D(G)$, $u = o(e)$ and $v = t(e)$ are called the *origin* and *terminus* of e, respectively. Furthermore, the arc $e^{-1} = (v, u)$ is the *inverse* of $e = (u, v)$.

A *path* $P = (e_1, \ldots, e_n)$ of *length* n in G is a sequence of $e_1, \ldots, e_n$ such that $e_i \in D(G), t(e_i) = o(e_{i+1})(1 \leq i \leq n-1)$. Set $|P| = n$. Furthermore, set $o(P) = o(e_1), t(P) = t(e_n)$. Then P is called an $(o(P), t(P))$*-path*. A path $P = (e_1, \cdots, e_n)$ has a *backtracking* if $e_{i+1}^{-1} = e_i$ for some $i = 1, \ldots, n-1$. A path $P = (e_1, \ldots, e_n)$ is called a *cycle* if $o(e_1) = t(e_n)$.

Two cycles $C_1 = (e_1, \cdots, e_n)$ and $C_2 = (e'_1, \cdots, e'_n)$ is equivalent if $e'_i = e_{i+k}$ $(i = 1, \ldots, n)$ for some $k \in \mathbf{N}$, where the subscripts are considered in mod n. Let $[C]$ be the equivalence class containing C. Let B^r be the cycle obtained by going r times around a cycle B. Such a cycle is called a *power* of B. A cycle C is *reduced* if both C and C^2 have no backtracking. Furthermore, a cycle C is *prime* if it is not a power of a strictly smaller cycle. Note that each equivalence class of prime, reduced cycles of a graph G corresponds to a unique primitive conjugacy class of the fundamental group $\pi_1(G, v)$ of G at a vertex v of G.

Definition 3 (Sunada, 1986) *The* Ihara zeta function *of a graph G is a function of $u \in \mathbb{C}$ with $|u|$ sufficiently small, defined by*

$$\mathbf{Z}(G, u) = \prod_{[C]} (1 - u^{|C|})^{-1},$$

where $[C]$ runs over all equivalence classes of prime, reduced cycles of G([38,39]).

2 Determinant expression of Ihara type for the Ihara zeta function by the terminologies of graph theory

2.1 Ihara Theorem

Let G be a connected graph n vertices $v_1, \ldots, v_n$ and m edges. Then the *adjacency matrix* $\mathbf{A}(G) = (a_{ij})_{1 \leq i,j \leq n}$ of G is defined as follows

$$a_{ij} = \begin{cases} 1 & \text{if } v_i v_j \in E(G) \text{ (or } (v_i, v_j) \in D(G)), \\ 0 & \text{otherwise,} \end{cases}$$

Furthermore, the *degree* $\deg v = \deg_G v = |\{v_j \mid v_i v_j \in E(G)\}|$ of a vetex v of G is the number of edges incident to v. A graph G is k*-regular* if $\deg v = k$ for each vertex $v \in V(G)$. For a integer $r \in \mathbf{N}$, let N_r be the number of reduced cycles of length r in G.

Theorem 2 (Ihara, 1966) *Let G be a connected $(q+1)$-regular graph with n vertices and m edges. Then the Ihara zeta function $\mathbf{Z}(G, u)$ of G is given as follows:*

$$\mathbf{Z}(G, u) = (1 - u^2)^{-(m-n)} \det(\mathbf{I}_n - \mathbf{A}(G)u + qu^2\mathbf{I}_n)^{-1} \quad (3)$$

$$= \exp\left(\sum_{k \geq 1} \frac{N_k}{k} u^k\right). \quad (4)$$

The right side of (3) is the *graph theoretic version of determinant expression of Ihara type* for the Ihara zeta function. Furthermore, (4) is the *exponential generating function* for the Ihara zeta function.

Example

Let $G = K_3$ be the complete graph (or the triangle) with three vertices v, w, z. Set $e = (v, w)$, $f = (w, z)$ and $g = (z, v)$. Then G is 2-regular. Furthermore, all equivalence classes of prime, reduced cycles in G are $[C], [C^{-1}]$, where $C = (e, f, g)$ and $C^{-1} = (e^{-1}, g^{-1}, f^{-1})$. By the definition of the Ihara zeta function, we have

$$\mathbf{Z}(G, u)^{-1} = (1 - u^{|C|})(1 - u^{|C^{-1}|}) = (1 - u^3)^2.$$

Furthermore we have

$$\mathbf{A}(G) = \begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{bmatrix}$$

and $m = n = 3$, $q = 1$. By Ihara Theorem, we have

$$\begin{aligned} \mathbf{Z}(G, u)^{-1} &= (1 - u^2)^{3-3} \det(\mathbf{I}_3 - u\mathbf{A}(G) + u^2\mathbf{I}_3) \\ &= \det \begin{bmatrix} 1 + u^2 & -u & -u \\ -u & 1 + u^2 & -u \\ -u & -u & 1 + u^2 \end{bmatrix} \\ &= (1 + u^2)^3 - 2u^3 - 3u^2(1 + u^2) = (1 - u^3)^2. \end{aligned}$$

By

$$\exp(\sum_{k \geq 1} \frac{N_k}{k} u^k) = (1 - u^3)^{-2},$$

we have

$$\sum_{k \geq 1} \frac{N_k}{k} u^k = \log(1 - u^3)^{-2} = 2(u^3 + \frac{u^6}{2} + \frac{u^9}{3} + \cdots) = \frac{6}{3}u^3 + \frac{6}{6}u^6 + \frac{6}{9}u^9 + \cdots .$$

Thus,

$$N_3 = N_6 = N_9 = \ldots = 6,\ N_k = 0(k \not\equiv 0\ mod\ 3).$$

Next, we state the properties of the Ihara zeta function of a regular graph G.

I. rationality.

By Theorem 2, the Ihara zeta function $\mathbf{Z}(G, u)$ is a reciprocal of a polynomial.

II. functional equation([37,40]).

Let

$$\Lambda_G(u) = (1 - u^2)^{n/2+r-1}(1 - q^2u^2)^{n/2}\mathbf{Z}(G, u),$$

where $n = |V(G)|$, $m = |E(G)|$ and $r = m - n + 1$. Then we have

$$\Lambda_G(u) = (-1)^n \Lambda_G(\frac{1}{qu}).$$

III. An analogue of the Riemann hypothesis[28,29]).

Let G be a $(q + 1)$-regular graph. If $s = \sigma + it$, $\mathbf{Z}(G, q^{-s}) = 0$ and $\mathrm{Re}(s) \in (0, 1)$, then

$$\mathrm{Re}(s) = \frac{1}{2}.$$

It is known that G satisfies an analogue of the Riemann hypothesis if and only if G is a Ramanujan graph.

Here, a $(q+1)$-regular graph G is *Ramanujan* if G satisfies the following condition:

$$\lambda \neq \pm(q+1) \Rightarrow |\lambda| \leq 2\sqrt{q}$$

for each eigenvalue λ of $\mathbf{A}(G)$.

2.2 Determinant expression of Ihara type for the Ihara zeta function of a general graph

Let G be a connected graph with n vertices and m edges. Then the *degree matrix* $\mathbf{D} = (d_{uv})$ is the $n \times n$ diagonal matrix defined as follows:

$$d_{uv} = \begin{cases} \deg u & \text{if } u = v, \\ 0 & \text{otherwise,} \end{cases}$$

Furthermore, two $2m \times 2m$ matrices $\mathbf{B} = \mathbf{B}(G) = ((\mathbf{B})_{e,f})_{e,f \in D(G)}$ and $\mathbf{J}_0 = \mathbf{J}_0(G) = ((\mathbf{J}_0)_{e,f})_{e,f \in D(G)}$ are given as follows:

$$(\mathbf{B})_{e,f} = \begin{cases} 1 & \text{if } t(e) = o(f), \\ 0 & \text{otherwise,} \end{cases} \quad (\mathbf{J}_0)_{e,f} = \begin{cases} 1 & \text{if } f = e^{-1}, \\ 0 & \text{otherwise.} \end{cases}$$

Then the matrix $\mathbf{B} - \mathbf{J}_0$ is called the *edge matrix* of G.

The graph theoretical versions of determinant expression for the Ihara zeta function are given as follows([4,18]).

Theorem 3 (Hashimoto; Bass) *For a connected graph G,*

$$\begin{aligned} &\mathbf{Z}_G(u)^{-1} = \det(\mathbf{I}_{2m} - u(\mathbf{B} - \mathbf{J}_0)) \\ = \ &(1-u^2)^{m-n} \det(\mathbf{I}_n - u\mathbf{A}(G) + u^2(\mathbf{D} - \mathbf{I}_n)) = \exp(-\textstyle\sum_{k \geq 1} \frac{N_k}{k} u^k), \end{aligned}$$

where $m = |E(G)|, n = |V(G)|$, and N_k is the number of reduced cycles of length k in G.

The first determinant expression is called *Hasimoto type*, and the second one is called *Ihara type*.

Example

Let G be a connected graph with four vertices v, w, x, y and five edges vw, vx, vy, wx, xy. Then we have

$$\mathbf{A}(G) = \begin{bmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{bmatrix}, \mathbf{D} = \begin{bmatrix} 3 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 2 \end{bmatrix}.$$

Since there are an infinitely many equivalence classes of prime, reduced cycles in G, we can not obtain an explicit formula for the Ihara zeta function of G by using the definition of the Ihara zeta functiion. By Theorem 3, we have

$$\begin{aligned} &\mathbf{Z}(G,u)^{-1} = (1-u^2)^{5-4} \det(\mathbf{I}_4 - u\mathbf{A}(G) + u^2(\mathbf{D} - \mathbf{I}_4)) \\ = \ &\det \begin{bmatrix} 1+2u^2 & -u & -u & -u \\ -u & 1+u^2 & -u & 0 \\ -u & -u & 1+2u^2 & -u \\ -u & 0 & -u & 1+u^2 \end{bmatrix} \\ = \ &(1-u^2)(1-u)(1+u^2)(1+u+2u^2)(1-u^2-2u^3). \end{aligned}$$

Furthermore,

$$\sum_{k\geq 1} \frac{N_k}{k} u^k = 4u^3 + 2u^4 + 4u^6 + 4u^7 + \cdots .$$

Thus,

$$N_3 = 12,\ N_4 = 8,\ N_5 = 0,\ N_6 = 24,\ N_7 = 28, \ldots .$$

3 Definition of the second weighted zeta function as a generalization of the Ihara zeta function

3.1 Definition of the second weighted zeta function

Let G be connected graph with n vertices and m edges. Then an $n \times n$ matrix $\mathbf{W}(G) = (w_{uv})$ is given as follows:

$$w_{uv} = \begin{cases} \textit{nonzero complex number} & \text{if } (u,v) \in D(G), \\ 0 & \text{otherwise.} \end{cases}$$

The matrix $\mathbf{W}(G)$ is the *weighted matrix* of G. Set $w(u,v) = w_{uv},\ u,v \in V(G)$ and $w(e) = w_{uv},\ e = (u,v) \in D(G)$.

Furthermore, we define a function $\tilde{w} : D'G) \times D(G) \longrightarrow \mathbb{C}$ as follows:

$$\tilde{w}(e,f) = \begin{cases} w(f) & \text{if } t(e) = o(f) \text{ and } f \neq e^{-1}, \\ w(f) - 1 & \text{if } f = e^{-1}, \\ 0 & \text{otherwise.} \end{cases}$$

Then, for a cycle $C = (e_1, e_2, \ldots, e_r)$, let

$$w_C = \tilde{w}(e_1,e_2)\tilde{w}(e_2,e_3)\cdots\tilde{w}(e_{r-1},e_r)\tilde{w}(e_r,e_1).$$

Definition 4 (Sato, 2007) *The* second weighted zeta function *of a graph G is defined as follows:*

$$\mathbf{Z}_1(G,w,u) = \prod_{[C]} (1 - w_C u^{|C|})^{-1},$$

where $[C]$ runs over all equivalence classes of prime cycles in G([33]).

If $w = \mathbf{1}$, i.e., $w(e) = 1$ for each $e \in D(G)$, then the second weighted zeta function is equal to the Ihara zeta function:

$$\mathbf{Z}_1(G,w,u) = \mathbf{Z}(G,u).$$

If a cycle C has a backtracking, then we have $w_C = 0$.

3.2 Determinant expression of Ihara type for the second weighted zeta function

The determinant expression of Ihara type for the second weighted zeta function is given as follows([33]):

Theorem 4 (Sato, 2007) *Let G be connected graph with n vertices and m edges, and $\mathbf{W}(G)$ a weighted matrix of G. Then the reciprocal of the second weighted zeta function of G is*

$$\mathbf{Z}_1(G,w,u)^{-1} = (1-u^2)^{m-n} \det(\mathbf{I}_n - u\mathbf{W}(G) + u^2(\mathbf{D}_w - \mathbf{I}_n)),$$

where the matrix $\mathbf{D}_w = (d_{uv})$ *is an* $n \times n$ *diagonal matrix with*

$$d_{uu} = \sum_{o(e)=u} w(e).$$

Example
Let $G = K_3$ be the complete graph with three vertices v, w, z and

$$\mathbf{W}(G) = \begin{bmatrix} 0 & a & b \\ c & 0 & d \\ p & q & 0 \end{bmatrix}.$$

Since there are an infinitely many equivalence classes of prime cycles in G, we can not obtain an explicit formula for the second weighted zeta function of G by using the definition of the second weighted zeta functiion. By Theorem 4, we have

$$\mathbf{Z}_1(G, w, u)^{-1} = (1-u^2)^{3-3} \det(\mathbf{I}_3 - u\mathbf{W}(G) + u^2(\mathbf{D}_w - \mathbf{I}_3))$$

$$= \det \begin{bmatrix} 1+(a+b-1)u^2 & -au & -bu \\ -cu & 1+(c+d-1)u^2 & -du \\ -pu & -qu & 1+(p+q-1)u^2 \end{bmatrix}$$

$$= 1 + (\alpha+\beta+\gamma - bp - ac - dq)u^2 - (adp + bcq)u^3$$

$$+ (\alpha\beta + \beta\gamma + \gamma\alpha - bp\beta - ac\gamma - dq\alpha)u^4 + \alpha\beta\gamma u^6,$$

where $\alpha = a+b-1$, $\beta = c+d-1$ and $\gamma = p+q-1$.

Next, we state one remark.

We present the determinant expression of Hashimoto type for the second weighted zeta function([33]). Let G be connected graph with n vertices and m edges, and $\mathbf{W}(G)$ a weighted matrix of G. Then a $2m \times 2m$ matrix $\mathbf{B}_w = \mathbf{B}_w(G) = (\mathbf{B}^{(w)}_{e,f})_{e,f \in D(G)}$ is given as follows:

$$\mathbf{B}^{(w)}_{e,f} = \begin{cases} w(f) & \text{if } t(e) = o(f), \\ 0 & \text{otherwise.} \end{cases}$$

Then

Theorem 5 (Sato, 2007) *Let* G *be connected graph with* n *vertices and* m *edges, and* $\mathbf{W}(G)$ *a weighted matrix of* G*. Then the determinant expression of Hashimoto type for the second weighted zeta function of* G *is*

$$\mathbf{Z}_1(G, w, u)^{-1} = \det(\mathbf{I}_{2m} - u(\mathbf{B}_w - \mathbf{J}_0)).$$

4 The results Emms et al from viewpoint of graph isomorphism problem

4.1 Historical background of quantum walk

Quantum walk was introduced from three fields:

1. *Quantum probability theory* : 1988, Gudder [16];
2. *Quantum cellular automaton* : 1996, Meyer [30];

3. *Quantum computer* :

   2000, Nayak and Vishwanath [31] ;

   2001, Ambainis, Bach, Nayak, Vishwanath and Watrous [2];

   2001, Aharonov, Ambainis, Kempe and Vazirani [1].

In the above articles, *discrete-time quantum walk* was introduced and *its properties* were studied.

In 2002, Childs, Farhi and Gutmann [5] defined *continuous quantum walk.*

In 2002, Professor Konno [23] presented *the limit theorem* of *two-state quantum walk on* $\mathbb{Z}$. Konno distribution is quite different from the normal distribution.

Next, we state historical background of graph isomorphism problem related to quantum walk.

1. In 2006, Emms, Hancock, Severini and Wilson [9] gave spectra for the *Grover (transition) matrix* (the time evolution matrix of Grover walk) of a graph and *its positive support* etc. Furthermore, they proposed a *conjecture* for *graph isomorphism problem* of *strongly regular graphs.*
2. In 2008, Emms [8] defined a *discrete-time quantum walk (Grover walk)* on a graph by using the Grover matrix.
3. In 2011, Ren, Aleksic, Emms, Wilson and Hancock [32] showed that the transpose of the positive support of the Grover matrix is equal to the *edge matrix* used in the determinant expression of the Ihara zeta function.
4. In 2012, Konno and Sato [25] presented the characteristic polynomial of the Grover matrix and its positive support by using determinant expressions of Ihara type for the Ihara zeta function and the second weighted zeta function, and directly obtained spectra for them .

4.2 Konno distribution

We consider a *two-state quantum walk on* $\mathbb{Z}$, that is, a discrete-time quantum walk which the particle moves at each time step either one unit to the right or the left(see [24]).

For each $k \in \mathbb{Z}$, we consider the *state*

$$\psi_k = \begin{bmatrix} \alpha_k \\ \beta_k \end{bmatrix} \in \mathbb{C}^2.$$

This is considered as an "inner state" of a particle. Here,

$$\sum_{k=-\infty}^{\infty} ||\psi_k||^2 = \sum_{k=-\infty}^{\infty} (|\alpha_k|^2 + |\beta_k|^2) = 1$$

Then ψ_k and α_k, β_k are called the *qubit state* and the *probability amplitudes* of k, respectively.

Next, we consider an unitary matrix

$$\mathbf{U} = \begin{bmatrix} a & b \\ c & d \end{bmatrix}.$$

Then $|a|^2 + |b|^2 = |b|^2 + |c|^2 = 1, \bar{b} + c\bar{d} = 0, c = -\Delta\bar{b}, d = \Delta\bar{a} (\Delta = ad - bc)$. As an analogue of the probabilities p,q of a random walk on $\mathbb{Z}$, we consider

$$\mathbf{P} = \begin{bmatrix} a & b \\ 0 & 0 \end{bmatrix}, \mathbf{Q} = \begin{bmatrix} 0 & 0 \\ c & d \end{bmatrix}.$$

The equation $\mathbf{U} = \mathbf{P} + \mathbf{Q}$ corresponds to $1 = p + q$, and $\mathbf{P}, \mathbf{Q}$ are non-commutative versions for p, q.

Furthermore, let

$$\psi_k^n = \begin{bmatrix} \alpha_k^n \\ \beta_k^n \end{bmatrix}$$

be the qubit state of the position $k (k = 0, \pm 1, \pm 2, \ldots)$ at time $n (n = 1, 2, \ldots)$. Then we define the *time evolution* for quantum walk on $\mathbb{Z}$ as follows:

$$\psi_k^n = \mathbf{P}\psi_{k+1}^{n-1} + \mathbf{Q}\psi_{k-1}^{n-1}.$$

For brevity, let the *initial qubit state* $(n = 0)$ be given as follows:

$$\psi_0^0 = \phi = \begin{bmatrix} \alpha \\ \beta \end{bmatrix} \in \mathbf{C}^2, \psi_k^0 = \begin{bmatrix} 0 \\ 0 \end{bmatrix} (k \neq 0).$$

where $||\phi||^2 = |\alpha|^2 + |\beta|^2 = 1$. We consider quantum walk stating at the origin of $\mathbb{Z}$ with the qubit state ϕ at $n = 0$.

In the case of $n = 1$, we have

$$\psi_1^1 = \mathbf{P}\psi_2^0 + \mathbf{Q}\psi_0^0 = \begin{bmatrix} a & b \\ 0 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ c & d \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \begin{bmatrix} 0 \\ c\alpha + d\beta \end{bmatrix},$$

$$\psi_{-1}^1 = \mathbf{P}\psi_0^0 + \mathbf{Q}\psi_{-2}^0 = \begin{bmatrix} a & b \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ c & d \end{bmatrix} \begin{bmatrix} 0 \\ 0 \end{bmatrix} = \begin{bmatrix} a\alpha + b\beta \\ 0 \end{bmatrix}.$$

If $k \neq \pm 1$, then, since $k \pm 1 \neq 0$,

$$\psi_k^1 = \mathbf{P}\psi_{k+1}^0 + \mathbf{Q}\psi_{k-1}^0 = \begin{bmatrix} a & b \\ 0 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ c & d \end{bmatrix} \begin{bmatrix} 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}.$$

In the case of $n = 2$, we have

$$\psi_0^2 = \mathbf{P}\psi_1^1 + \mathbf{Q}\psi_{-1}^1 = \begin{bmatrix} a & b \\ 0 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ c\alpha + d\beta \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ c & d \end{bmatrix} \begin{bmatrix} a\alpha + b\beta \\ 0 \end{bmatrix} = \begin{bmatrix} b(c\alpha + d\beta) \\ c(a\alpha + b\beta) \end{bmatrix}.$$

Similarly, we have

$$\psi_2^2 = \begin{bmatrix} 0 \\ d(a\alpha + b\beta) \end{bmatrix}, \psi_{-2}^2 = \begin{bmatrix} a(c\alpha + d\beta) \\ 0 \end{bmatrix}.$$

If $k \neq 0, \pm 2$, then, since $k \pm 1 \neq \pm 1$,

$$\psi_k^2 = \begin{bmatrix} 0 \\ 0 \end{bmatrix}.$$

Now, let X_n be the quantum walk at time n. Then the *probability* which there exits a particle in the position k at time n is defined as follows:

$$P(X_n = k) = ||\psi_k^n||^2 = |\alpha_k^n|^2 + |\beta_k^n|^2.$$

Example (Hadamard walk)

If

$$\mathbf{U} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}, \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ i \end{bmatrix},$$

then this discrete-time quantum walk is called the *Hadamard walk*. Then the probabilities are given as follows:

n/k	-2	-1	0	1	2	v
0	0	0	1	0	0	1
1	0	1/2	0	1/2	0	1
2	1/4	0	1/2	0	1/4	1

In general, Konno [23] presented the weak limit theorem with respect to $n \to \infty$ for two-state quantum walk on $\mathbb{Z}$.

Theorem 6 (Konno) *Let*

$$\begin{bmatrix} \alpha \\ \beta \end{bmatrix} (|\alpha|^2 + |\beta|^2 = 1).$$

For quantum walk stating at the origin of $\mathbb{Z}$ *with the above qubit state* ϕ *at* $n = 0$*,*

$$\frac{X_n}{n} \longrightarrow Z \ (n \to \infty) \ (weak\ convergence),$$

that is,

$$\lim_{n\to\infty} P(u \leq \frac{X_n}{n} \leq v) = \int_u^v \frac{\sqrt{1-|a|^2}}{\pi(1-z^2)\sqrt{|a|^2-z^2}} \{1 - (|\alpha|^2 - |\beta|^2 + \frac{a\alpha\bar{b}\bar{\beta} + \bar{a}\bar{\alpha}b\beta}{|a|^2} z\} dz.$$

Example (Hadamard walk) In the Hadamard walk,

$$\lim_{n\to\infty} P(u \leq \frac{X_n}{n} \leq v) = \int_u^v \frac{1}{\pi(1-z^2)\sqrt{1-z^2}} dz.$$

4.3 Discrete-time Grover walk on a graph

Let G be a connected graph with m edges. Then we state a discrete-time Grover walk over $D(G)$ along Emms [8].

For each arc $e = (u, v) \in D(G)$, we indicate the *pure state* $\vec{x}_e = \vec{x}_{uv}$ such that $\{\vec{x}_e \mid e \in D(G)\}$ is a normal orthogonal system on the Hilbert space $\mathbb{C}^{2m}$. The *transition* from an arc (u, v) to an arc (w, x) occurs if $v = w$. The *state* of quantum walk is defined as follows:

$$\psi = \sum_{(u,v)\in D(G)} \alpha_{uv}\vec{x}_{uv}, \ \alpha_{uv} \in \mathbb{C}.$$

The *probability* which there exists a particle in the arc (u, v) is given as follows:

$$P(\vec{x}_e) = \alpha_{uv}\overline{\alpha_{uv}}.$$

Here,

$$\sum_{(u,v)\in D(G)} \alpha_{uv}\overline{\alpha_{uv}} = 1.$$

In the classical discrete-time random walk, the relation of the states ψ_{t+1}, ψ_t is given by

$$\psi_{t+1} = \mathbf{U}\psi_t$$

through some unitary matrix $\mathbf{U}$. Similarly, the time evolution of quantum walk over $D(G)$ is defined by using the *Grover matrix* $\mathbf{U} = (U_{(w,x),(u,v)})$(see [15]):

$$U_{(w,x),(u,v)} = \begin{cases} 2/\deg v & \text{if } v = w, x \neq u, \\ 2/\deg v - 1 & \text{if } v = w, x = u, \\ 0 & \text{otherwise} \end{cases}$$

This quantum walk is called the *(discrete-time) Grover walk* on G. Note that the Grover matrix is unitary.

Example

Let G be the graph with $V(G)=\{u,v,w,x\}$ and $D(G)=\{(u,v),(v,u),(v,w),(w,v),(v,x),(x,v)\}$. Furthermore, we arrange arcs of $D(G)$ as follows: $(u,v),(v,u),(w,v),(v,w),(x,v),(v,x)$. Then the Grover matrix $\mathbf{U}$ is

$$\mathbf{U}=\begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ -1/3 & 0 & 2/3 & 0 & 2/3 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 2/3 & 0 & -1/3 & 0 & 2/3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 2/3 & 0 & 2/3 & 0 & -1/3 & 0 \end{bmatrix}$$

If $\psi_t = a\vec{x}_{uv} - b\vec{x}_{wv}$ $(a^2+b^2=1)$, then $\psi_{t+1}=\mathbf{U}\psi_t = a\mathbf{U}\vec{x}_{uv} - b\mathbf{U}\vec{x}_{wv}$. Since $\vec{x}_{uv}={}^t(100000)$,$\vec{x}_{wv}={}^t(001000)$,

$$\begin{aligned}\psi_{t+1} &= a^t(0\ -1/3\ 0\ 2/3\ 0\ 2/3) - b^t(0\ 2/3\ 0\ -1/3\ 0\ 2/3) \\ &= (-1/3a-2/3)\vec{x}_{vu} + (2/3a+1/3b)\vec{x}_{vw} + 2/3(a-b)\vec{x}_{vx},\end{aligned}$$

where $(-1/3a-2/3)^2+(2/3a+1/3b)^2+4/9(a-b)^2=a^2+b^2=1$.

4.4 A conjecture for graph isomorphism problem

Two graphs G, H are *isomorphic* $(G \cong H)$ if there exists a bijection $f : V(G) \longrightarrow V(H)$ such that $uv \in E(G)$ if and ony if $f(u)f(v) \in E(H)$. Then the graph isomorphism problem is given as follows:

Problem 1 *For two graphs G and H, determine whether $G \cong H$.*

It is known that this problem is very difficult. Also, there is the following problem.

Problem 2 *For any two graphs G and H, is there an invariant $f(G)$ of graphs such that $G \cong H$ if and only if $f(G)=f(H)$?*

Until now, such invariants are not found.

The characteristic polynomial $\Phi(G;\lambda)=\det(\lambda\mathbf{I}-\mathbf{A}(G))$ of a graph G is not an invariant for problem 2. It is known that there exist G,H such that $\Phi(G;\lambda)=\Phi(H;\lambda)$ and $G \ncong H$([3]). Furthermore, the Ihara zeta function of a graph is not an invariant for problem 2. There exist G,H such that $\mathbf{Z}(G,u)=\mathbf{Z}(H;u)$ and $G \ncong H$([6]).

Through quantum walk, decision algorithms for graph isomorphism and new approach for graph isomorphism problem are proposed by Shiau, Joynt and Coopersmith [36], Emms, Severini, Wilson,and Hancock [10], Douglas and Wang [7], Gamble, Friesen, Zhou, Joynt and Coopersmith [11]. Furthermore, Emms, Hancock, Severini and Wilson [9] proposed a conjecture which is partially affirmative for problem 2.

For a real square matrix $\mathbf{A}=(a_{ij})$, the *positive support* $\mathbf{A}^+=(a^+_{ij})$ of $\mathbf{A}$ is defined as follows:

$$a^+_{ij} = \begin{cases} 1 & \text{if } a_{ij}>0, \\ 0 & \text{otherwise.} \end{cases}$$

Then

Conjecture 1 (Emms, Hancock, Severini and Wilson, 2006) *Let* G, H *be* strongly regular graphs *with same parameters. Then*

$$G \cong H \Leftrightarrow Spec((\mathbf{U}(G)^3)^+) = Spec((\mathbf{U}(H)^3)^+),$$

where $Spec(\mathbf{F})$ *is the set of spectra (eigenvalues) of a square matrix* $\mathbf{F}$*, and* $\mathbf{U}(G)$ *is the Grover matrix of* G*.*

A graph G is a *strongly regular graph* with *parameters* n, k, λ, μ or an (n, k, λ, μ)*-graph* if the following four conditions are satisfied([14]):

1. $|V(G)| = n$G
2. For each vertex v of G, $\deg v = k$G
3. any two adjacent vertices u, v are adjacent to the λ common verticesG
4. any non-adjacent vertices x, y are adjacent to the μ common vertices. @

Note that an (n, k, λ, μ)-graph is a k-regular graph. For example, the complete bipartite graph $K_{n,n}$ is a $(2n, n, 0, n)$-graph.

The above conjecture does not hold for regular graphs. There are 4-regular graphs G, H with 14 vertices such that $G \ncong H$ and $Spec((\mathbf{U}(G)^3)^+) = Spec((\mathbf{U}(H)^3)^+)$([9]). By using a computer, Emms et al [10] showed that the conjecture holds for some strongly regular graphs. If the conjecture holds, then $Spec((\mathbf{U}(G)^3)^+)$ or $\Phi((\mathbf{U}(G)^3)^+; \lambda)$ are invariants for problem 2 in a small family of graphs (possibly infinite set).

5 Konno-Sato Theorem

5.1 Konno-Sato Theorem

Now, we give an explicit formula for the characteristic polynomial of the Grover matrix of a graph([25]).

Let G be a connected graph with n vertices and m edges. Then an $n \times n$ matrix $\mathbf{T}(G) = (T_{uv})_{u,v \in V(G)}$ is defined as follows:

$$T_{uv} = \begin{cases} 1/(\deg u) & \text{if } (u, v) \in D(G), \\ 0 & \text{otherwise.} \end{cases}$$

This matrix $\mathbf{T}(G)$ is the transition matrix of the simple random walk on G.

Then

Theorem 7 (Konno and Sato, 2012) *Let* G *be a connected graph with* n *vertices* $v_1, \ldots, v_n$ *and* m *edges. Then the characteristic polynomial for the Grover matrix* $\mathbf{U}$ *of* G *is given by*

$$\det(\lambda \mathbf{I}_{2m} - \mathbf{U}) = (\lambda^2 - 1)^{m-n} \det((\lambda^2 + 1)\mathbf{I}_n - 2\lambda \mathbf{T}(G)) \tag{5}$$

$$= \frac{(\lambda^2 - 1)^{m-n} \det((\lambda^2 + 1)\mathbf{D} - 2\lambda \mathbf{A}(G))}{d_{v_1} \cdots d_{v_n}}. \tag{6}$$

Proof. By Theorem 4. Q.E.D.

By Theorem 7.(5), we express spectra of the Grover matrix $\mathbf{U}$ by using those of $\mathbf{T}(G)$([9]).

Corollary 1 (Emms, Hancock, Severini and Wilson, 2006) *Let* G *be a connected graph with* n *vertices and* m *edges. Then the spectra of the Grover matrix* $\mathbf{U}$ *are given as follows:*

1. $2n$ *eigenvalues:*

$$\lambda = \lambda_T \pm i\sqrt{1-\lambda_T^2},$$

where λ_T *are spectra of* $\mathbf{T}(G)$*;*

2. $2(m-n)$ *eigenvalues:* ± 1 *with same multiplicities.*

Proof. By Theorem 7.(5), we have

$$\det(\lambda \mathbf{I}_{2m} - \mathbf{U}) = (\lambda^2 - 1)^{m-n} \prod_{\lambda_T \in Spec(\mathbf{T}(G))} (\lambda^2 + 1 - 2\lambda_T \lambda).$$

Solving $\lambda^2 + 1 - 2\lambda_T\lambda = 0$, we obtain

$$\lambda = \lambda_T \pm i\sqrt{1-\lambda_T^2},$$

and so the result follows. Q.E.D.

By Theorem 7.(6), we obtain the following result for a regular graph(c.f., [9]).

Corollary 2 (Emms, Hancock, Severini and Wilson, 2006) *Let* G *be a connected* k*-regular graph with* n *vertices and* m *edges. Then the spectra of the Grover matrix* $\mathbf{U}$ *are given as follows:*

1. $2n$ *eigenvalues:*

$$\lambda = \frac{\lambda_A \pm i\sqrt{k^2-\lambda_A^2}}{k},$$

where λ_A *are spectra of the adjacency matrix* $\mathbf{A}(G)$ *of* G*;*

2. $2(m-n)$ *eigenvalues:* ± 1 *with same multiplicities.*

Proof. At first, we have $\mathbf{D} = k\mathbf{I}_n$. By Theorem 7.(6),

$$\det(\lambda \mathbf{I}_{2m} - \mathbf{U}) = \frac{(\lambda^2 - 1)^{m-n}}{d_{v_1} \cdots d_{v_n}} \prod_{\lambda_A \in Spec(\mathbf{A}(G))} (k\lambda^2 + k - 2\lambda_A \lambda).$$

Solving $k\lambda^2 + k - 2\lambda_A\lambda = 0$, we obtain

$$\lambda = \frac{\lambda_A \pm i\sqrt{k^2-\lambda_A^2}}{k},$$

and so, the result follows. Q.E.D.

5.2 Positive support of the Grover matrix

At fist, we state the relation between the Ihara zeta function and the Grover matrix([32]).

Theorem 8 (Ren, Aleksic, Emms, Wilson and Hancock) *Let* G *be a connected graph with* n *vertices and* m *edges. Suppose that the minimum degree* $\delta(G)$ *of* G *is not less than 2. Then the transpose of the positive support of the Grover matrix* $\mathbf{U}$ *of* G *is equal to the edge matrix appeared in the determinant expression of Hashimoto type for the Ihara zeta function of* G*:*

$$\mathbf{B} - \mathbf{J}_0 = ({}^t\mathbf{U})^+.$$

By Theorem 3 and Theorem 8, we obtain the characteristic polynomial for the positive support $\mathbf{U}^+$ of the Grover matrix of a graph.

Theorem 9 *Let G be a connected graph with n vertices and m edges. Then the characteristic polynomial for the positive support $\mathbf{U}^+$ of the Grover matrix of a graph is given by*

$$\det(\lambda \mathbf{I}_{2m} - \mathbf{U}^+) = (\lambda^2 - 1)^{m-n} \det((\lambda^2 - 1)\mathbf{I}_n - \lambda \mathbf{A}(G) + \mathbf{D}).$$

Proof. By Theorem 3 and Theorem 8,

$$\begin{aligned}\det(\mathbf{I}_{2m} - u\mathbf{U}^+) &= \det(\mathbf{I}_{2m} - u({}^t\mathbf{B} - {}^t\mathbf{J}_0)) \\ &= \det(\mathbf{I}_{2m} - u(\mathbf{B} - \mathbf{J}_0)) \\ &= (1-u^2)^{m-n} \det(\mathbf{I}_n - u\mathbf{A}(G) + u^2(\mathbf{D} - \mathbf{I}_n)).\end{aligned}$$

Now, set $u = 1/\lambda$. Then we have

$$\det\left(\mathbf{I}_{2m} - \frac{1}{\lambda}\mathbf{U}^+\right) = \left(1 - \frac{1}{\lambda^2}\right)^{m-n} \det\left(\mathbf{I}_n - \frac{1}{\lambda}\mathbf{A}(G) + \frac{1}{\lambda^2}(\mathbf{D} - \mathbf{I}_n)\right).$$

Thus,

$$\det(\lambda \mathbf{I}_{2m} - \mathbf{U}^+) = (\lambda^2 - 1)^{m-n} \det((\lambda^2 - 1)\mathbf{I}_n - \lambda \mathbf{A}(G) + \mathbf{D}).$$

Q.E.D.

By Theorem 9, we express spectra for the positive support $\mathbf{U}^+$ of the Grover matrix of a regular graph by using those of the adjacency matrix $\mathbf{A}(G)$(c.f., [9]).

Corollary 3 (Emms, Hancock, Severini and Wilson, 2006) *Let G be a connected k-regular graph with n vertices and m edges. Then the spectra of the positive support $\mathbf{U}^+$ of the Grover matrix $\mathbf{U}$ are given as follows:*

1. *$2n$ eigenvalues:*
$$\lambda = \frac{\lambda_A}{2} \pm i\sqrt{k - 1 - \lambda_A^2/4},$$
where λ_A are spectra of the adjacency matrix $\mathbf{A}(G)$ of G;
2. *$2(m-n)$ eigenvalues: ± 1 with same multiplicities.*

Proof. By Theorem 9,

$$\begin{aligned}\det(\lambda \mathbf{I}_{2m} - \mathbf{U}^+) &= (\lambda^2 - 1)^{m-n} \det((\lambda^2 + k - 1)\mathbf{I}_n - \lambda \mathbf{A}(G)) \\ &= (\lambda^2 - 1)^{m-n} \textstyle\prod_{\lambda_A \in Spec(\mathbf{A}(G))} (\lambda^2 + k - 1 - \lambda_A \lambda).\end{aligned}$$

Solving $\lambda^2 + k - 1 - \lambda_A \lambda = 0$, we have

$$\lambda = \frac{\lambda_A}{2} \pm i\sqrt{k - 1 - \lambda_A^2/4}.$$

Q.E.D.

5.3 Positive support of the square of the Grover matrix

At fist, we state the structure theorem for the positive support $(\mathbf{U}^2)^+$of the square of the Grover matrix $\mathbf{U}$ of a graph([12]).

Theorem 10 (Godsil and Guo, 2011) *Let G be a connected k-graph with m edges, and suppose that $k > 2$. Then*

$$(\mathbf{U}^2)^+ = (\mathbf{U}^+)^2 + \mathbf{I}_{2m}.$$

By Theorem 9 and Theorem 10, we obtain the characteristic polynomial for the positive support $(\mathbf{U}^2)^+$ the square of the Grover matrix of a graph([19]).

Theorem 11 (Higuchi, Konno, Sato and Segawa, 2013) *Let G be a connected k-graph with n vertices and m edges, and suppose that $k > 2$. Then the characteristic polynomial for the positive support $(\mathbf{U}^2)^+$ of the square of the Grover matrix of a graph is given by*

$$\det(\lambda \mathbf{I}_{2m} - (\mathbf{U}^2)^+) = (\lambda - 2)^{2m-2n} \det((k-2+\lambda)^2 \mathbf{I}_n - (\lambda - 1)\mathbf{A}(G)^2).$$

By Theorem 11, we express spectra for the positive support $(\mathbf{U}^2)^+$ of the square of the Grover matrix of a regular graph by using those of the adjacency matrix $\mathbf{A}(G)$(c.f., [9]).

Corollary 4 (Emms, Hancock, Severini and Wilson, 2006) *Let G be a connected k-regular graph with n vertices and m edges. Suppose that $k > 2$. Then the spectra of the positive support $(\mathbf{U}^2)^+$ of the square of the Grover matrix $\mathbf{U}$ are given as follows:*

1. *$2n$ eigenvalues:*
$$\lambda = \frac{\lambda_A^2 - 2k + 4}{2} \pm i\lambda_A \frac{\sqrt{4k - 4 - \lambda_A^2}}{2},$$
where λ_A are spectra of the adjacency matrix $\mathbf{A}(G)$ of G;

2. *$2(m-n)$ eigenvalues:* 2.

Proof. By Theorem 11, we have

$$\begin{aligned}
\det(\lambda \mathbf{I}_{2m} - (\mathbf{U}^2)^+) &= (\lambda - 2)^{2m-2n} \det((k-2+\lambda)^2 \mathbf{I}_n - (\lambda - 1)\mathbf{A}(G)^2) \\
&= (\lambda - 2)^{2m-2n} \prod_{\lambda_A \in Spec(\mathbf{A}(G))} ((k-2+\lambda)^2 - (\lambda - 1)\lambda_A^2).
\end{aligned}$$

Similarly to Corollaries 1,2,3, we obtain the result. Q.E.D.

Now, we state a reason why $Spec(\mathbf{U})$, $Spec(\mathbf{U}^+)$, $Spec((\mathbf{U}^2)^+)$ are not invariants for problem 2.

Let G, H be two (n, k, λ, μ)-graph (strongly regular graph). Then it is known that

$$Spec(\mathbf{A}(G)) = Spec(\mathbf{A}(H)) = \{k, \theta, \tau\},$$

where
$$\theta = \frac{(\lambda - \tau) + \sqrt{\Delta}}{2}, \tau = \frac{(\lambda - \tau) + \sqrt{\Delta}}{2}, \Delta = (\lambda - \tau)^2 + 4(k - \mu)$$

and the multiplicities of θ, τ are determined by n, k, λ, μ([14]).

By Corollaries 1,2,3 and 4, the eigenvalues of $\mathbf{U}, \mathbf{U}^+, (\mathbf{U}^2)^+$ is decided by the eigenvalues of the adjacency matrix. Thus,

$$Spec(\mathbf{U}(G)) = Spec(\mathbf{U}(H)), Spec(\mathbf{U}(G)^+) = Spec(\mathbf{U}(H)^+), Spec((\mathbf{U}(G)^2)^+) = Spec((\mathbf{U}(H)^2)^+).$$

Therefore, $Spec(\mathbf{U})$, $Spec(\mathbf{U}^+)$, $Spec((\mathbf{U}^2)^+)$ can not decide whether $G \cong H$.

By this fact, Emms et al [9] explored the spectra of the positive support of the cube of the Grover matrix.

5.4 Positive support of the cube of the Grover matrix

We present the structure theorem of $(\mathbf{U}^3)^+$ as Theorem 10.

Let G be a graph. Then the *girth* $g(G)$ of G is the minimum length of prime, reduced cycles in G. Then the structure theorem of $(\mathbf{U}^3)^+$ is given as follows([19]):

Theorem 12 (Higuchi, Konno, Sato and Segawa, 2013) *Let G be a connected k-graph with n vertices and m edges, and suppose that $k > 2$ and $g(G) > 4$. Then*

$$(\mathbf{U}^3)^+ = (\mathbf{U}^+)^3 + {}^t\mathbf{U}^+.$$

If $\lambda \geq 1$ for an (n, k, λ, μ)-graph G, then we have $g(G) = 3$, and so we can not use Theorem 12 to resolve the conjecture.

Anyway we present an explicit formula for the characteristic polynomial for the positive support of the cube of the Grover matrix under the same conditions as Theorem 12([27]).

Theorem 13 (Konno, Sato and Segawa, 2014) *Let G be a connected k-graph with n vertices and m edges, and suppose that $k > 2$ and $g(G) > 4$. Then the characteristic polynomial for the positive support $(\mathbf{U}^3)^+$ of the cube of the Grover matrix of G is given by*

$$\det(\lambda \mathbf{I}_{2m} - (\mathbf{U}^3)^+) = (\lambda - 4)^{m-n} \det((\lambda^2 \mathbf{I}_n - \lambda(\mathbf{A}^3 - (3k-4)\mathbf{A})$$

$$+ \quad (\mathbf{A}^4 - k^2\mathbf{A}^2 + 2(k-1)(k^2 - 2k + 2)\mathbf{I}_n),$$

where $\mathbf{A} = \mathbf{A}(G)$.

Thus,

Corollary 5 (Segawa, 2014) *Let G be a connected k-graph with n vertices and m edges, and suppose that $k > 2$ and $g(G) > 4$. Then the spectra of the positive support $(\mathbf{U}^3)^+$ of the cube of the Grover matrix $\mathbf{U}$ are given as follows([34]):*

1. *$2n$ eigenvalues:*

$$\lambda = \frac{1}{2}\{\lambda_A(\lambda_A^2 - 3k + 4)$$

$$\pm \sqrt{\lambda_A^6 - 2(3k-2)\lambda_A^4 + (13k^2 - 24k + 16)\lambda_A - 8(k-1)(k^2 - 2k + 2)}\},$$

   where λ_A are spectra of the adjacency matrix $\mathbf{A}(G)$ of G;

2. *$2(m-n)$ eigenvalues: ± 2.*

From the above result, an approach for the conjecture is as follows: Let G, H be (n, k, λ, μ)-graphs and $k > 2$. If there are such graphs G, H such that $G \ncong H$ and $g(G) > 4$, $g(H) > 4$, then the conjecture does not hold.

But, there exist at most four strongly regular graphs G with $g(G) > 4$.

5.5 A counterexample for the conjecture

In 2015, Godsil, Guo and Myklebust [13] gave a counterexample for the conjecture.

The *generalized quadrangle of order* (s, t) is an incidence structure such that

1. Any point belongs to $(s + 1)$ lines, and
2. any line contains $(t + 1)$ points.

Then it is known that the *line intersection graph* of the generalized quadrangle of order (s, t) is a $((t+1)(st+1), s(t+1), t-1, s+1)$-*graph (strongly regular graph).* Furthermore, it is known that *there exist two non-isomorphic generalized quadrangles of order* $(5^2, 5)$:

$$H(3, 5^2), \ FTWKB(5).$$

Now, let X and Y be the line intersection graph of $H(3, 5^2)$ and $FTWKB(5)$, respectively. Then X, Y are $(756, 130, 4, 26)$-graphs and $X \ncong Y$.

Godsil et al [13] showed that

$$Spec((\mathbf{U}(X)^3)^+) = Spec((\mathbf{U}(Y)^3)^+).$$

by using computer. Thus, Emms et al conjecture does not hold !!

5.6 Further remark

Recently, we consider Konno problem([25]):

Problem 3 (Konno, 2012) *For $\forall n \in \mathbb{N}$, determine the characteristic polynomial for the positive support $(\mathbf{U}^n)^+$ of the n th power of the Grover matrix of a graph G.*

Konno problem is a quite difficult problem.
Konno problem is equivalent to the following problem:

Problem 4 *For $\forall n \in \mathbb{N}$, determine a determinant expression of Ihara type for the following zeta function:*

$$\zeta_k(G,u) = \det(\mathbf{I}_{2m} - u(\mathbf{U}^k)^+),\ m = |E(G)|.$$

Let G be a connected r-regular graph with n vertices and m edges. By Theorems 11 and 13, we obtain the following results:

1. $r = 2$:

$$\zeta_2(G,u)^{-1} = (1-2u)^{2m-2n} \det((1+u(r-2))^2\mathbf{I}_n - (1-u)\mathbf{A}(G)^2)\ (r > 2);$$

2. $r = 3$:

$$\zeta_3(G,u)^{-1} = (1-4u^2)^{m-n} \det(\mathbf{I}_n - u(\mathbf{A}^3 - (3r-4)\mathbf{A})$$

$$+ \quad u^2(\mathbf{A}^4 - k^2\mathbf{A}^2 + 2(r-1)(r^2-2r+2)\mathbf{I}_n)(r > 2, g(G) > 4),$$

where $\mathbf{A} = \mathbf{A}(G)$.

Furthermore, we can give the structure theorem for the positive support $(\mathbf{U}^n)^+$ of the n th power of the Grover matrix of a graph G under some conditions([26]).

Theorem 14 (Konno, Sato and Segawa, 2018) *Let G be a connected r-graph with $g(G) > 2k-2$. Then*

$$(\mathbf{U}^k)^+ = \sum_{j=0}^{k}(\epsilon_j(\mathbf{U}^+)^j + \tau_j\mathbf{J}_0(\mathbf{U}^+)^j) + \sum_{j=0}^{k-1}(\epsilon_{-j}{}^t(\mathbf{U}^+)^j + \tau_{-j}{}^t(\mathbf{J}_0(\mathbf{U}^+)^j)),$$

where $\epsilon_j, \tau_j = 0, 1$ $(j = 0, \pm 1, \ldots, \pm(k-1), k)$.

This structure theorem is not explicit.

Corollary 6 (Konno, Sato and Segawa, 2018)

$$(\mathbf{U}^4)^+ = \mathbf{J}_0(\mathbf{U}^+)^2\mathbf{J}_0 + \mathbf{I} + (\mathbf{U}^+)^4,$$

$$(\mathbf{U}^5)^+ = \begin{cases} \mathbf{J}_0(\mathbf{U}^+)^3\mathbf{J}_0 + \mathbf{J}_0\mathbf{U}^+\mathbf{J}_0 + \mathbf{U}^+ + (\mathbf{U}^+)^5 & \text{if } 3 \le r \le 6, \\ \mathbf{J}_0(\mathbf{U}^+)^3\mathbf{J}_0 + (\mathbf{U}^+)^2\mathbf{J}_0 + \mathbf{J}_0\mathbf{U}^+\mathbf{J}_0 + \mathbf{U}^+ & \\ \qquad +\mathbf{J}_0(\mathbf{U}^+)^2 + (\mathbf{U}^+)^5 & \text{if } r \ge 7, \end{cases}$$

$$(\mathbf{U}^6)^+ = \begin{cases} \mathbf{J}_0(\mathbf{U}^+)^4\mathbf{J}_0 + \mathbf{J}_0(\mathbf{U}^+)^2\mathbf{J}_0 + \mathbf{I} + (\mathbf{U}^+)^2 + (\mathbf{U}^+)^6 & \text{if } r = 3, 4, \\ \mathbf{J}_0(\mathbf{U}^+)^4\mathbf{J}_0 + (\mathbf{U}^+)^3\mathbf{J}_0 + \mathbf{J}_0(\mathbf{U}^+)^2\mathbf{J}_0 + \mathbf{I} + (\mathbf{U}^+)^2 & \\ \qquad +\mathbf{J}_0(\mathbf{U}^+)^3 + (\mathbf{U}^+)^6 & \text{if } 5 \le r \ge 11, \\ \mathbf{J}_0(\mathbf{U}^+)^4\mathbf{J}_0 + (\mathbf{U}^+)^3\mathbf{J}_0 + \mathbf{I} + (\mathbf{U}^+)^2 + \mathbf{J}_0(\mathbf{U}^+)^3 & \\ \qquad +(\mathbf{U}^+)^6 & \text{if } r \ge 12. \end{cases}$$

From now on, we shall study Konno problem, and then we would like to consider the relation between the Ihara zeta function and quantum walk.

Finally, we state a few comments. We challenge the conjecture for graph isomorphism problem by using the Ihara zeta function, and our attempt is mistake. From this approach for the conjecture, we show that the Ihara zeta function is very strong, and we are sure that the Ihara zeta function makes a new field in the world of quantum walk. From now on, the Ihara zeta function will be developed in various fields more and more.

Acknowledgment

I would like to thank Professor Masanobu Kaneko very much for giving a variable chance to talk in Ihara80. Furthermore, I would like to thank Professor Hideaki Morita for many valuable comments and many helpful suggestions.

References

[1] D. Aharonov, A. Ambainis, J. Kempe, and U. V. Vazirani, Quantum walks on graphs, Proc. of the 33rd Annual ACM Symposium on Theory of Computing, 50-59, 2001.

[2] A. Ambainis, E. Bach, A. Nayak, A. Vishwanath and J. Watrous, One-dimensional quantum walks, Proc. of the 33rd Annual ACM Symposium on Theory of Computing, 37-49, 2001.

[3] G. A. Baker, Drum shapes and isospectral graphs, J. Math. Phys. **7** (1966), 2238-2243.

[4] H. Bass, The Ihara-Selberg zeta function of a tree lattice, Internat. J. Math. **3** (1992), 717-797.

[5] A. M. Childs, E. Farhi and S. Gutmann, An example of the difference between quantum and classical random walks, Quantum Inform. Process. **1** (2002), 35-43.

[6] Y. Cooper, Properties determined by the Ihara zeta function of a graph, Electronic J. Combin. **16** (2009), R84.

[7] B. L. Douglas and J. B. Wang, Classically efficient graph isomorphism algorithm using quantum walks, arXiv: 0705.2531.

[8] D. M. Emms, Analysis of graph structure using quantum walks, Ph. D. Thesis, University of York, 2008.

[9] D. M. Emms, E. R. Hancock, S. Severini and R. C. Wilson, A matrix representation of graphs and its spectrum as a graph invariant, Electronic J. Combin. **13** (2006), R34.

[10] D. M. Emms, S. Severini, R. C. Wilson and E. R. Hancock, Coined quantum walks lift the cospectrality of graphs and trees, Pattern Recognit. **42** (2009), 1988-2002.

[11] J. K. Gamble, M. Friesen, D. Zhou, R. Joynt and S. N. Coopersmith, Two-particle quantum walks applied to the graph isomorphism problem, Phys. Rev. A **81** (2010), 52313.

[12] C. Godsil and K. Guo, Quantum walks on regular graphs and eigenvalues, Electron. J. Combin. **18** (2011), paper 165, 9 pp.

[13] C. Godsil, K. Guo and T. G. J. Myklebust, Quantum walks on generalized quadrangles, Electron. J. Combin. **24** (2017), paper 4.16, 6 pp.

[14] C, Godsil and G. Royle, *Algebraic Graph Theory*, Springer, New York, 2001.

[15] L. Grover, A first quantum mechanical algorithm for database search, Proc. of the 28 th Annual ACM Symposium on Theory of Computing, 212-219, 1996.

[16] S. P. Gudder, *Quantum Probability*, Academic Press Inc. CA, 1988.

[17] K. Hashimoto, Zeta Functions of Finite Graphs and Representations of p-Adic Groups, Adv. Stud. Pure Math. Vol. 15, pp. 211-280, Academic Press, New York (1989).

[18] K. Hashimoto, On the zeta- and L-functions of finite graphs, Internat. J. Math. **1** (1990), 381-396.

[19] Yu. Higuchi, N. Konno, I. Sato and E. Segawa, A note on the discrete-time evolutions of quantum walk on a graph, J. Math-for-Ind. **5B** (2013), 103-109.

[20] Y. Ihara, Algebraic curves *mod* $\mathcal{B}$ and arithmetic groups, Proc. Sympos. in Pure Math. IX. Boulder, Colo. 265-271, 1965.

[21] Y. Ihara, Discrete subgroups of $PGL(k_{\mathcal{B}})$, Proc. Sympos. in Pure Math. IX. Boulder, Colo. 272-278, 1965.

[22] Y. Ihara, On discrete subgroups of the two by two projective linear group over p-adic fields, J. Math. Soc. Japan **18** (1966), 219-235.

[23] N. Konno, Quantum random walks in one dimension, Quantum Inform. Process. **1** (2002), 345-354.

[24] H. Konno, *Mathematics of Quantum Walk*(in Japanese), Sangyo Tosho, 2008.

[25] N. Konno and I. Sato, On the relation between quantum walks and zeta functions, Quantum Inform. Process. **11(2)** (2012), 341-349.

[26] N. Konno, I. Sato and E. Segawa, Phase measurement of quantum walks: application to structure theorem of the positive support of the Grover walk, arXiv:1801.06209.

[27] N. Konno, I. Sato and E. Segawa, A zeta function related to the transition matrix of the discrete-time quantum walk on a graph, preprint.

[28] A. Lubotzky, Cayley graphs: Eigenvalues, expanders and random walks, in: Surveys in Combinatorics, in: London Math. Soc. Lecture Note Ser., vol. 218, Cambridge Univ. Press, Cambridge, 1995, pp. 155-189.

[29] A. Lubotzky, R. Phillips, and P. Sarnak, Ramanujan graphs, Combinatorica **8** (1988), 261-277.

[30] D. Meyer, From quantum cellular automata to quantum lattice gases, J. Statist. Phys. **85** (1996), 551-574.

[31] A. Nayak, and A. Vishwanath, Quantum walk on the line, DIMACS Technical report, 2000-43, 2000.

[32] P. Ren, T. Aleksic, D. Emms, R.C. Wilson and E.R. Hancock, Quantum walks, Ihara zweta functions and cospectrality in regular graphs, Quantum Inform. Process. **10** (2011), 405-417.

[33] I. Sato, A new Bartholdi zeta function of a graph. Int. J. Algebra **1** (2007), 269–281.

[34] E. Segawa, private communication, 2014.

[35] J. -P. Serre, *Trees,* Springer-Verlag, New York, 1980.

[36] S. -Y. Shiau, R. Joynt and S. N. Coopersmith, Physically-motivated dynamical algorithms for the graph isomorphism problem, Quantum Inform. Comput. **5** (2005), 492-506.

[37] H. M. Stark and A. A. Terras, Zeta functions of finite graphs and coverings, Adv. Math. **121** (1996), 124-165.

[38] T. Sunada, L-Functions in Geometry and Some Applications, in Lecture Notes in Math., Vol. 1201, pp. 266-284, Springer-Verlag, New York (1986).

[39] T. Sunada, *Fundamental Groups and Laplacians*(in Japanese), Kinokuniya Shoten, 1988.

[40] A. Terras, *Zeta functions of graphs: A Stroll through the Garden*, Cambridge studies in advanced mathematics, Vol. 128, Cambridge University Press, Cambridge (2011).